Abstract

In this thesis, we study hyperbolic problem with volume preservation, where a free boundary appears. This problem can be obtained by examining the motion of a droplet on plane. In this phenomenon, the drop is divided into two interacting parts: a film representing the surface of the drop, and the fluid inside. The motion of the liquid is described by equation of fluid dynamics (Euler equations). The film, which determines a (moving) boundary for the liquid inside, is considered to be the graph of a scalar function. Free boundary, volume constraint and contact angle are three main features of the model of the film. The underlying surface, on which the droplet rests, plays the role of an obstacle to the motion and gives rise to free boundary. Moreover, the volume preservation constraint is obtained from assumption that the volume of the drop does not change. Finally, there is a positive contact angle on the boundary of the region where the drop touches the surface. The hyperbolic free boundary problem with volume conservation constraint is solved by discrete Morse flow method. Moreover, a model taking into account both the surface and the liquid body is solved by combining discrete Morse flow and smoothed particle hydrodynamics method.

1 Introduction

In this work, the content follows: in Section 2, we derive governing equation of motion of film representing the surface of the droplet. In the next section, we use discrete Morse flow to construct an approximation solution to the governing equation (hyperbolic free boundary problem with volume conservation constraint). Then, we introduce the couple model which combines the above governing equation with Euler equations for the fluid inside film as shown in Section 4. Section 5 presents some numerical results for the moving of a droplet on the plane and inclined plane.

2 The model of film

In this work, $\theta \leq 90^0$ is our consistent consideration. Then we can describe the surface as a scalar function $u : (0, T) \times \Omega \to \mathbf{R}$, where $(0, T)$ is the time interval and Ω is the domain where the motion is considered. The surface, on which the drop rests, plays the role of an obstacle. The boundary of the set $\{u > 0\}$ is the free boundary.

The film model equation is derived based on Hamilton's principle. Adopting a basic form of surface energy, the action of the film is written as

$$J(u) = \int_0^T \int_\Omega \Big(\frac{\sigma}{2} u_t^2 \chi_{u>0} - \frac{\gamma_g}{2} |\nabla u|^2 - R^2 \chi_\varepsilon(u) - \frac{1}{2} \rho g u^2 \chi_{u>0}\Big) dx dt,$$

Here σ is area density of the surface, γ_g and R^2 describe the surface tension properties of the material, ρ is the fluid density, $\chi_{u>0}$ is the characteristic function of the set $\{u > 0\}$, and $\chi_\varepsilon(u) \in C^2(\mathbf{R})$ is a smoothing of $\chi_{u>0}$.

Searching for its stationary points, first variation gives

$$\chi_{u>0} \sigma u_{tt} = \gamma_g \Delta u - \rho g u \chi_{u>0} - R^2 \chi'_\varepsilon(u) + \lambda. \tag{1}$$

where

$$\lambda = \frac{1}{V} \int_\Omega \Big(\gamma_g |\nabla u|^2 + \rho g u^2 \chi_{u>0} + R^2 u \chi'_\varepsilon(u) + \sigma u_{tt} u \chi_{u>0}\Big) dx.$$

In the case of a droplet on inclined plane with angle α, above equation becomes

$$\chi_{u>0} \sigma u_{tt} = \gamma_g \Delta u - f \chi_{u>0} - R^2 \chi'_\varepsilon(u) + \lambda, \tag{2}$$

where $f = \rho g(u \cos\theta - x_1 \sin\theta)$, here x_1 is the horizontal axis, and

$$\lambda = \frac{1}{V} \int_\Omega \Big(\gamma_g |\nabla u|^2 + \rho g(u^2 \cos\alpha - u x_1 \sin\alpha) \chi_{u>0} + R^2 u \chi'_\varepsilon(u) + \sigma u_{tt} u \chi_{u>0}\Big) dx.$$

3 Numerical method

In this content, we use discrete Morse flow method to construct an approximation solution to equation of film motion.
First, we fix a large number $N > 0$, determine the time step $h = T/N$ and consider the approximate shapes of the film u_n at time levels $t_n = nh, n = 0, 1, 2, .., N$. The shape u_0 is given as the initial condition $u(0, x)$ and u_1 can be approximated using u_0 and initial velocity as $u_1 = u_0 + v_0 h$, here $v_0 = u_t(0, x)$. The approximate solution u_n on further time levels $t = nh$ for $n = 2, 3, .., N$, to be the minimizer of the following functional

$$J_n(u) = \int_\Omega \left(\sigma \frac{|u - 2u_{n-1} + u_{n-2}|^2}{2h^2} \chi_{u>0} + \frac{\gamma_g}{2} |\nabla u|^2 + R^2 \chi_\varepsilon(u) + \rho g u^2 \chi_{u>0} \right) dx. \quad (3)$$

in the admissible set

$$K := \left\{ u \in H_0^1(\Omega); \int_\Omega u \chi_{u>0} = V \right\}$$

Calculating the first variation of J_n under volume conservation condition, we find that minimizers of the functional J_n construct an approximation solution to (1).
In order to obtain a minimizer $u_n, n = 2, 3, .., N$ of functional $J_n(u)$ we use minimizing algorithm following:

1. Set up initial condition u_0, v_0, and we have $u_1 = u_0 + hv_0$,
2. For $n = 1, 2, .., N$, determine u_{n+1} using the following procedure:
   (a) $a^1 = u_n$
   (b) For $k = 1, 2, .., K_n$
      i. compute the gradient $p_k = \nabla_u J_n(a^k)$,
      ii. search for minimizer (using the steepest descent method and bisection method) $\widetilde{a}^{k+1}$ of J_n in the direction $-p_k$,
      iii. $\widetilde{a}^{k+1} = max(\widetilde{a}^{k+1}, 0)$
      iv. project a^{k+1} on the volume-constraint hyperplane: $a^{k+1} = P(\widetilde{a}_{k+1})$,
      v. if $|J_n(a^k) - J_n(a^{k+1})| < \xi$ then $K_n = k + 1$ else $k = k + 1$
   (c) $u_{n+1} = a^{K_n}$

In this algorithm, the $J_n(a^k)$ is calculated by using finite element method for space discretization. Furthermore, minimizers are determined by the steepest descent method combined with bisection method (step ii).

Taking as an example, we consider the behaviour of the film of a droplet pinned by the solid surface (Figure.1). We use equation (1) with the parameter as

$$\sigma = 1, \gamma_g = 1, \rho = 1, R^2 = 1.2, \varepsilon = 0.03, h = 7.5 \times 10^{-4}$$

and this example is calculated under Dirichlet boundary condition.

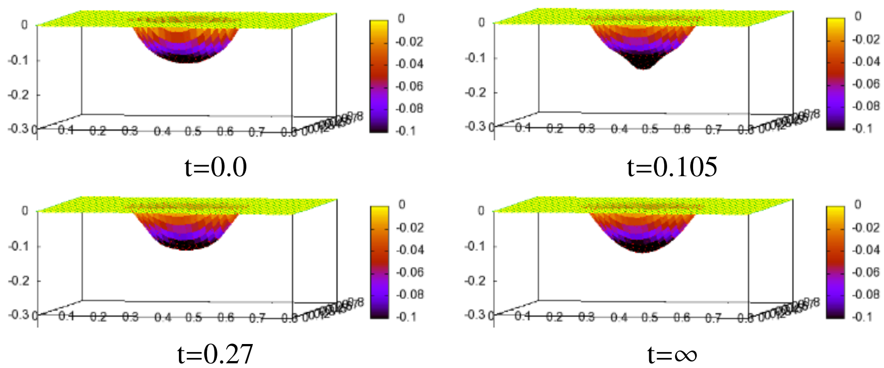


Figure 1: *A droplet hanging on the plane.*

4 Couple model

In this part, we consider a couple model which combines the motion of film with fluid motion inside film.
From the assumption, the domain of fluid flow is given as:

$$\Omega_f(t) = \{(x_1, x_2, z) \in \mathbf{R}^3; z \in (0, u(x_1, x_2))\} \tag{4}$$

In this domain, we propose the motion of fluid following the equations:
Conservation of mass

$$\frac{D\rho}{Dt} + \rho \nabla . \mathbf{v} = 0, \text{ in } \cup_{t\in(0,T)} \Omega_f(t) \times \{t\}, \tag{5}$$

Conservation of momentum

$$\frac{D\mathbf{v}}{Dt} = -\frac{1}{\rho} \nabla P + \mathbf{g}, \text{ in } \cup_{t\in(0,T)} \Omega_f(t) \times \{t\}, \tag{6}$$

where $\mathbf{v}$ is the velocity, P is the pressure and $\mathbf{g}$ is the gravitation force.
The pressure is determined by

$$P = c^2(\rho - \rho_0)$$

where c is the artificial sound speed and ρ_0 is the reference density.

In order to achieve the model of the droplet motion, we consider one more outer force against the surface - the pressure force pushing the film from the inside. The pressure force per unit area is written as $P\mathbf{n}$, where

$$\mathbf{n} = \frac{1}{\sqrt{1 + |\nabla u|^2}}(-u_{x_1}, -u_{x_2}, 1)$$

is the unit outer normal vector of the surface. Therefore, $P(x, u, t)$ is the net force which is applied to the film. Thus, the equation (2) becomes

$$\chi_{u>0}\sigma u_{tt} = \gamma_g \Delta u - f\chi_{u>0} - R^2\chi_\varepsilon'(u) + \lambda, \tag{7}$$

where $f = \rho g(u\cos\theta - x_1 \sin\theta) - P|_{z=u}$, and

$$\lambda = \frac{1}{V}\int_\Omega \Big(\gamma_g|\nabla u|^2 + \rho g(u^2 \cos\alpha - ux_1 \sin\alpha)\chi_{u>0} - uP|_{z=u} + R^2 u\chi_\varepsilon'(u) + \sigma u_{tt} u\chi_{u>0}\Big)dx.$$

For the fluid flow, we impose $\mathbf{v} = 0$ on the plane $z = 0$, $\mathbf{v}(x, u, t) = (0, 0, u_t)$ on the film $z = u(x_1, x_2)$.
In summary, a model of the droplet motion is given as

$$\chi_{u>0}\sigma u_{tt} = \gamma_g \Delta u - f\chi_{u>0} - R^2\chi_\varepsilon'(u) + \lambda, \qquad \text{in } \Omega \times (0, T), \tag{8}$$

$$\frac{D\rho}{Dt} = -\rho\nabla.\mathbf{v}, \qquad \text{in } \cup_{t\in(0,T)} \Omega_f(t) \times \{t\}, \tag{9}$$

$$\frac{D\mathbf{v}}{Dt} = -\frac{1}{\rho}\nabla P + \mathbf{g}, \qquad \text{in } \cup_{t\in(0,T)} \Omega_f(t) \times \{t\}, \tag{10}$$

$$P = c^2(\rho - \rho_0), \qquad \text{in } \cup_{t\in(0,T)} \Omega_f(t) \times \{t\}, \tag{11}$$

$$\mathbf{v}|_{z=0} = 0, \mathbf{v}|_{z=u}(x, u, t) = (0, 0, u_t). \tag{12}$$

The whole system is solved by combining discrete Morse flow with smooth particle hydrodynamic method. At each time level $t = nh$, we have $u_n, \mathbf{x}_n$, and $\mathbf{v}_n$, from which we can find the new shape u_{n+1} of the film and the new position $\mathbf{x}_{n+1}$ of the fluid as follows:

1. Predict the shape of film u^* using the discrete Morse flow method without pressure force.

2. Determine position $\mathbf{x}_{n+1}$ and pressure P_{n+1} under region below u^*, using smoothed particle hydrodynamics method.

3. Determine the new shape u_{n+1} of the film, using the discrete Morse flow method with pressure force.

5 Numerical result

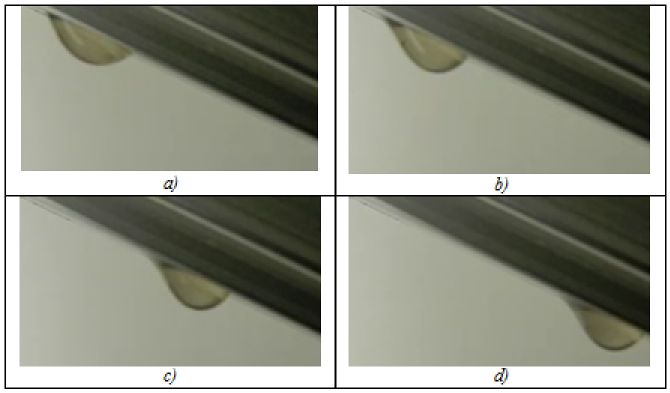


Figure 2: *A droplet lying under inclined plane (experiment).*

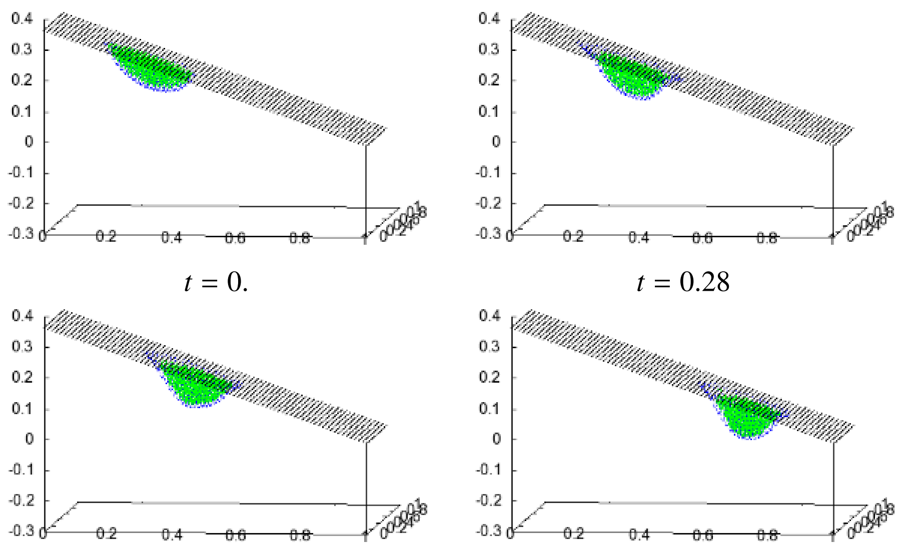
We use above procedure to simulate the motion of a droplet under inclined plane with angle $\alpha = 20^0$ (Figure. 2). The fluid inside the drop is represented by 1451 particles. The parameters of the equation (8) are given as

$$\sigma = 1, \gamma_g = 1., \rho = 3, R^2 = 1.65, \varepsilon = 0.04, h = 4 \times 10^{-4}.$$

By observing the numerical results (Figure 3), it can be seen that the shape of droplet oscillates and the volume of the droplet is precisely preserved while the droplet moves. In addition, all of particles representing the fluid are controlled well by the film of the droplet during the motion. This results show qualitative agrees with observations from the real experiments.

6 Conclusions

We have derived the hyperbolic free boundary problem with volume conservation constraint based on examining the motion of the surface of a droplet on plane or inclined plane. An approximation solution of this problem has been designed using the discrete Morse flow method. This method induced good numerical results, the droplet oscillates and its volume is precisely preserved. We have also presented a couple model for the moving droplet by combining the above hyperbolic problem for the film with the Euler equations for fluid filling film. In this case, the film plays as the moving boundary of the fluid and it always fills on role. Numerical result shows qualitative agreement with observed fact. Our future goal is quantitative comparison for this model.



$t = 0.$ $t = 0.28$

$t = 0.56$ $t = 1.12$

Figure 3: *A droplet lying under inclined plane (simulation), blue dots represent the film, green points represent the fluid inside the film and black dots represent the inclined plane.*

学位論文審査結果の要旨

Nguyen 氏は平成 22 年 10 月にベトナムメコン１０００プロジェクトの奨学生として金沢大学大学院自然科学研究科数物科学専攻博士後期課程に入学した。それ以来、双曲型自由境界問題の２次元数値解析方法の開発と、それと連成させる３次元流体方程式の粒子法によるソルバーの開発を行ってきた。この問題に対する物理的なモデルは「水面に浮かぶ泡の動力学」や「平面上の液滴の動力学」である。これは表面張力が主たる力となる問題で従来の粒子法では扱いづらい問題であった。本論文の主たるアイデアは、表面の膜を内部流体と切り離して取り扱い、体積保存制約条件・接触角などの要素を膜によって与えていることである。最終的に得られる方程式は退化双曲型となり、さらに自由境界をもつ問題となり数学的な解を得ることは困難である。同氏はこの問題を変分法に基づく離散勾配流法により数値解法の開発を行い、十分に実用的な結果を得た。流体内部については SPH 法による計算方法を開発した。膜を境界として取り扱い弱連成問題として双方の方程式を解いている。膜と粒子の相互作用では圧力を媒介としている。また、膜表面状に仮想粒子を用いて粒子の飛散を防いでいる。同氏は、自分で行った実験と数値計算を比較しており、その結果十分に実験を再現していると判断された。

Nguyen 氏はこれらを原著論文１報にまとめた。このことにより平成 25 年 8 月 1 日に開催された発表会とそれに引き続いて行われた審査会において本論文により博士（理学）の学位を授与するに値すると判断した。